

3-Amino-3-(naphthalen-1-yl)propanoic acid
100393-41-7 | DTXSID80377489

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 202 °C

Global applicability domain: Inside

Local applicability domain index: 5.14e-01

Confidence level: 5.19e-01

Nearest Neighbors from the Training Set

Image not found

2-Naphthalenecarboxylic acid, 3-amino-

Measured: 217

Predicted: 208

Image not found

Quinoline-4-carboxylic acid

Measured: 255

Predicted: 165

Image not found

8-Quinolinecarboxylic acid

Measured: 187

Predicted: 165

Image not found

N-Phenylanthranilic acid

Measured: 184

Predicted: 195

Image not found

2-Quinolinecarboxylic acid

Measured: 156

Predicted: 176